SINGLE-HOLE IN THE t-J MODEL: A VARIATIONAL MONTE CARLO STUDY

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ABSTRACT

We report results of variational Monte Carlo calculation for a hole in the t-J model on the square lattice. The analogy of this model with the one describing the motion of an impurity in a Bose fluid is shown. A Feynman-Cohen-type wave-function, similar to that describing the motion of a ^3He particle inside liquid ^4He, is used. Comparing our results for the 4×4 lattice case with exact diagonalization results, we find that the wave-function works well for $J/t > 1$. The single-hole energy $E(\mathbf{K})$ has been calculated for several values of J/t, on a 10×10 lattice. Its general features are in agreement with earlier calculations. We are currently working to introduce spin-hole-spin correlations in the wave-function, that we believe should improve the results for $J/t < 1$.

1. Introduction

The nearly half-filled, two-dimensional (2D) Hubbard model has been suggested [1] as an appropriate starting point for the study of superconducting copper oxides. The t-J model corresponds to the strong-coupling limit of the Hubbard model; however, it can also be derived from more general, and perhaps more realistic models [2 . Several attempts have been made to study the 2D t-J model in the presence of one or two holes, by using both analytical and numerical techniques. The problem of pairing of two holes has been studied on a small-size cluster [3], by exact diagonalization; it is found that a range of J/t exists for which pairing, induced by antiferromagnetic (AF) spin-correlations, might be possible. Much effort has been devoted in order to achieve a thorough understanding of the single-hole problem; theoretical predictions obtained for this case may lend themselves to a check against experimental results, for instance far-infrared studies of the reflectivity of lightly doped copper-oxide superconducting compounds (see, for instance, [8]). Some information has been produced [4,5,6,7] about certain features of the single-hole dispersion relation and the spectral function, where a quasiparticle peak has been found. The variational approach, which overcomes the limitations of dealing with small-size lattices, may provide both an analytical understanding of the nature of the correlations introduced by the hole and a deeper insight on the possibility of hole

pairing; additionally, it can be used further as a guiding function in a Green's Function Monte Carlo simulation, to determine the physics that is missing in the variational wave-function. In this work we have carried out a variational Monte Carlo (VMC) calculation for a single hole. The construction of the trial wave-function can be guided by the formal analogy between this problem and the one of the motion of an impurity in a Bose fluid, which was studied by Feynman and Cohen in 1956 [9]. Our variational wave-function works fairly well for $J/t > 1$, as it is shown by comparison with exact diagonalization results for the 4×4 lattice. We have calculated the single-hole energy dispersion curve $E(\mathbf{K})$ on a 10×10 lattice, for several values of J/t in the range where the wave-function works better; this curve reproduces several features that have been found in previous works.

2. The model

The t-J model is defined by the Hamiltonian

$$H = -t \sum_{<ij>\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + J_z \sum_{<ij>} (s^z_i s^z_j - \frac{1}{4}\hat{n}_i \hat{n}_j) + \frac{1}{2} J_{xy} \sum_{<ij>} (s^+_i s^-_j + s^-_i s^+_j), \qquad (1)$$

with $J_z = J_{xy} = J$. The first term represents electron (or, equivalently, hole) hopping from a lattice site to a nearest neighboring one, with no double occupancy, while the second and third term correspond to the AF spin-$\frac{1}{2}$ Heisenberg Hamiltonian, within an additive constant; we consider the case of one hole in an $N \times N$ lattice, and search for a suitable trial state for a variational Monte Carlo calculation. The Hamiltonian (1) conserves the value of the z-component of the total spin of the system. Thus, the eigenstates of (1) can be written as a superposition of configurations having a fixed number of "up" spins. Let us consider the Hilbert space of all possible states of the system, with N_u up-spins. A basis vector can be written as $|\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_{N_u} >$, with $\mathbf{R} \neq \mathbf{r}_1, \mathbf{r}_2, ... \mathbf{r}_{N_u}$, where $\mathbf{R}$ is the position of the hole and $\mathbf{r}_1, \mathbf{r}_2 ..., \mathbf{r}_{N_u}$ are the positions of the N_u up-spins. More precisely,

$$|\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2 ... \mathbf{r}_{N_u} >= s^+_{\mathbf{r}_1} s^+_{\mathbf{r}_2} ... s^+_{\mathbf{r}_{N_u}} |\mathbf{R}, F >, \qquad (2)$$

where the reference state $|\mathbf{R}, F >$ is the ferromagnetic aligned state with the hole at $\mathbf{R}$ and all the spins "down". The most general eigenstate of (1), having N_u up-spins, can be written as

$$|\Psi >= \sum_{\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N_u}} (-1)^{L(c)} \Psi(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N_u}) |\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N_u} >, \qquad (3)$$

where the sum runs over all possible positions of hole and up-spins. The phase factor $(-1)^{L(c)}$ depends on the spin configuration: $L(c)$ is the number of "up" spins in the odd (or even) sublattice. The amplitude $\Psi(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N_u})$ is symmetric under exchange of any two coordinates $\mathbf{r}_i, \mathbf{r}_j$, as it can be easily inferred from the commutation rule $[s^+_{\mathbf{r}_i}, s^+_{\mathbf{r}_j}] = 0$. Moreover, $\Psi(\mathbf{R}, ...\mathbf{r}_i ... \mathbf{r}_j ...) = 0$, if $\mathbf{r}_i = \mathbf{r}_j$ for any pair i, j as a result of $(s^+_{\mathbf{r}})^2 |\mathbf{R}, F >= 0$. Up-spins can be

therefore regarded as particles, namely as "hard-core" bosons. In this representation we can write down the eigenvalue equation $\hat{H}\Psi = \epsilon\Psi$ for the function $\Psi(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{N_u})$, with

$$\hat{H} = -\frac{\hbar^2}{2m_h}\tilde{\nabla}^2_{\mathbf{R}} - \frac{\hbar^2}{2m_b}\sum_1^{N_u}\tilde{\nabla}^2_{\mathbf{r}_i} + \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j) + \sum_i U(\mathbf{r}_i - \mathbf{R}) - t\sum_{<\mathbf{r}_i\mathbf{R}>}\hat{P}(\mathbf{r}_i, \mathbf{R}), \tag{4}$$

where $\epsilon = E + 3JN_u - 4t$, E being the ground state energy eigenvalue of (1), and $\tilde{\nabla}^2_{\mathbf{x}}\Psi(\mathbf{x}) \equiv \frac{\sum_{\mathbf{a}}(\Psi(\mathbf{x}+\mathbf{a})-\Psi(\mathbf{x}))}{a^2}$ is the Laplacian operator on the discrete square-lattice; a is a vector from a lattice site to a nearest neighboring one. $\hat{P}(\mathbf{r}, \mathbf{r}')$ is a two-"particle" exchange operator. The first two terms of the Hamiltonian are kinetic energy terms, one for the hole, whose "mass" is $m_h = \hbar^2 a^2/2t$, the other for the bosons introduced above, whose "mass" is $m_b = 2\hbar^2 a^2/J$. V_{ij} and U_i are interaction potentials between two bosons and a hole and a boson, featuring an infinite on-site repulsion; $V_{ij}(U_i)$ is equal to $J(J/2)$ for nearest-neighbor sites and zero otherwise. Apart from the fifth term, that we shall examine below, (4) is the lattice version of the Hamiltonian for an interacting boson lattice gas in which a foreign particle, in this case the hole, is moving. This is analogous to the problem of a ^3He atom moving inside a liquid ^4He background; we may therefore use a trial wave-function of the form proposed in [9]. The fifth term of the Hamiltonian (4), represents the exchange taking place between the hole and a nearest-neighboring boson; this exchange term is absent in the Hamiltonian studied in [9]. One could formally discretize the Hamiltonian for liquid ^4He with a ^3He impurity, according to the procedure first outlined by Matsubara and Matsuda [10], but such an exchange term would not arise. This term is not, then, merely a consequence of the discrete nature of the problem, but it rather expresses the possibility for a hole and a nearest-neighboring boson to interchange without involvement of a third or more particles. Because of that, unlike the case of ^3He atom inside a liquid ^4He background, hole motion inside the boson "fluid" does not necessarily cause a rearrangement of the fluid itself in the vicinity of the moving hole (backflow).

3. The variational wave-function

A general expression for the wave-function describing the motion of a ^3He impurity through liquid ^4He is :

$$\Psi = e^{i\mathbf{K}\cdot\mathbf{R}}\Phi_{\mathbf{i}}\Phi_{\mathbf{b}} \tag{5}$$

with

$$\Phi_{\mathbf{i}} = exp[-\frac{1}{2}(\sum_i u^{(2)}_{\mathbf{i}}(\mathbf{R}, \mathbf{r}_i) + \sum_{i<j} u^{(3)}_{\mathbf{i}}(\mathbf{R}, \mathbf{r}_i, \mathbf{r}_j) + ...)] \tag{5'}$$

and

$$\Phi_{\mathbf{b}} = exp[-\frac{1}{2}(\sum_{i<j} u^{(2)}_{\mathbf{b}}(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i<j<k} u^{(3)}_{\mathbf{b}}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + ...)] \tag{5''}$$

where $\mathbf{R}$ is the coordinate of the ^3He atom, $\mathbf{r}_i, \mathbf{r}_j, ...$ are the coordinates of the ^4He atoms. Φ_b describes correlations accounting for the hard-core repulsion between ^4He atoms while Φ_i describes the correlations between ^3He and ^4He atoms. $u^{(2)}$ are two-body correlation functions, $u^{(3)}$ three-body and so on. Our aim is to extend this wave-function to our problem. In this calculation we have only considered two-body correlations; we are currently investigating the effects of three-body correlations, associated with the $u^{(3)}$ terms [15]. For simplicity we now set $u_b^{(2)}(\mathbf{r}_i, \mathbf{r}_j) = u(\mathbf{r}_i, \mathbf{r}_j)$. In the Feynman-Cohen wave function [9], $u_i^{(2)}(\mathbf{r}, \mathbf{R}) = 2[g_1(\mathbf{K}, \mathbf{r} - \mathbf{R}) + ig_2(\mathbf{K}, \mathbf{r} - \mathbf{R})]$. ig_2 describes a backflow pattern around the foreign ^3He atom. In our case, it can also describe the exchange taking place between the hole, playing the role of ^3He, and a nearest-neighboring boson. We can now go back to spin variables, by using the identity $\hat{n}(\mathbf{r}) = s_{\mathbf{r}}^z + \frac{1}{2}$ where $\hat{n}(\mathbf{r})$ is the boson number operator at lattice site $\mathbf{r}$ (1 if there is an up-spin, zero otherwise); Φ_b, within a multiplicative constant, is given by

$$\Phi_b = exp(-\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} u(\mathbf{r}, \mathbf{r}')s_{\mathbf{r}}^z s_{\mathbf{r}'}^z), \tag{7}$$

where the sum now runs over all lattice sites. This is the Marshall wave-function for variational calculations on the spin-1/2 antiferromagnetic Heisenberg model [11,12,13]. We can treat the hole-boson term analogously, so that we end up with the following expression for $|\Psi_T>$, within a normalization constant:

$$|\Psi_T> = \sum_{\mathbf{R},c}(-1)^{L(c)}e^{i\mathbf{K}\cdot\mathbf{R}}exp[-\sum_{\mathbf{r}}(g_1(\mathbf{K}, \mathbf{r} - \mathbf{R}) + ig_2(\mathbf{K}, \mathbf{r} - \mathbf{R}))s_{\mathbf{r}}^z]$$

$$exp(-\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'} u(\mathbf{r}, \mathbf{r}')s_{\mathbf{r}}^z s_{\mathbf{r}'}^z)|\mathbf{R}, c> \tag{8}$$

where c is a generic spin configuration of the system. A similar wave-function was suggested in [6] as a resu.t of a perturbative expansion, in powers of t/J, of the so-called Ising limit of the Hamiltonian (1), obtained by setting $J_{xy} = 0$. Our approach is based upon the analogy of (1) with the Hamiltonian for the motion of an impurity in a Bose fluid. A similar wave-function, in the case of liquid ^4He, gives excitation energies for the phonon-maxon-roton spectrum that are accurate in the long-wavelength limit and $\sim$ 20% higher at intermediate momenta. However, it fails at higher momenta due to mode-mode coupling [14]. In the present paper, we neglect three-boson correlations in the wave-function, as well as boson-hole-boson correlations. We believe the introduction of such three-body correlations will improve the estimate of the hole energy with respect to the variational wave-function (8).

4. Results

The expression (8), represents the wave-function which we have implemented in our calculation. We have taken $u(\mathbf{r}, \mathbf{r}')$ to be the same as the one found in the variational treatment of spin-1/2 Heisenberg antiferromagnets ([13-14]);

it features the long-range tail $1/|\mathbf{r}-\mathbf{r}'|$ consistent with spin-wave theory. In general, $g_1(\mathbf{K},\mathbf{r})$ and $g_2(\mathbf{K},\mathbf{r})$ may be long-range functions. In our calculation, we have taken the functions $g_1(\mathbf{K},\mathbf{r})$ and $g_2(\mathbf{K},\mathbf{r})$ to be nonzero for nearest-neighbors only, and their values and signs were used as variational parameters; in general, their optimal values depend on $\mathbf{K}$. Unlike other quantities, the energy is not very sensitive to the tails of the wave-function. Boson-hole-boson and other hole-background correlations will be important in the large t/J limit; this is indeed the case in the Ising limit of (1), which corresponds to the motion of the hole inside a static background of spins [5]. We performed VMC calculations on 4×4 and 10×10 lattices with periodic boundary conditions. Metropolis algorithm with single-spin updates was used. Fig. 1 compares numerical results for the hole energy in the 4×4 lattice [4] with our variational results at $\mathbf{K} = (\pi/2, \pi/2)$, where the dispersion curve has its minimum, for both $g_1 = g_2 = 0$ (crosses) and the optimal g_1, g_2 (circles), for several values of J/t.

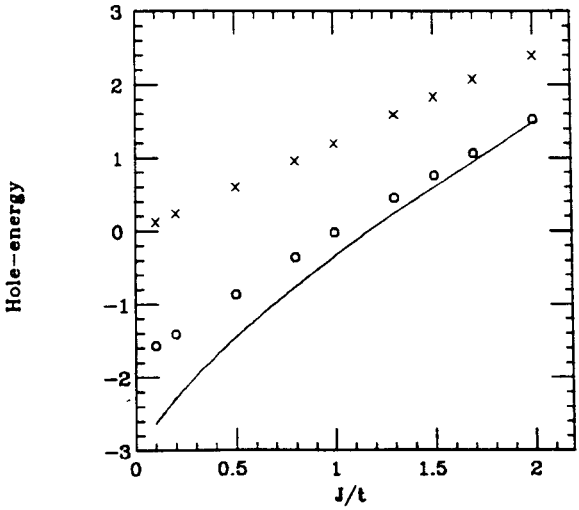

Fig.1. Hole energy in the 4×4 lattice. The solid line is the exact diagonalization result. Crosses refer to the variational results with $g_1 = g_2 = 0$, whereas circles represent variational results with the optimal g_1, g_2.

The case $g_1(\mathbf{K},\mathbf{r}) = g_2(\mathbf{K},\mathbf{r}) = 0$ corresponds to a state where hole hopping is neglected; switching on $g_1(\mathbf{K},\mathbf{r})$ and $g_2(\mathbf{K},\mathbf{r})$ improves significantly the ground state energy estimate for all values of J/t. The variational wave function works well when $J/t \geq 1$; similar results are found for the 10×10 lattice. In the regime where $J/t < 1$ the wave function can be improved by taking into account boson-hole-boson correlations. The function $E(\mathbf{K})$ was also computed for several values of J/t. A typical result is shown in Fig. 2-3 for $J/t = 1$. The curve features a minimum at $\mathbf{K} = (\pm\pi/2, \pm\pi/2)$, and attains its maximum value at $\mathbf{K} = (\pi, \pi)$. The effective mass of the hole is smaller in the direction $(0,0)$ to (π,π) than in the direction $(0,\pi)$ to $(\pi,0)$ (compare Fig.2 with Fig. 3). These results are in agreement with the qualitative statements made in [7].

It is possible that the hole dispersion curve is linear near the minimum, i.e. $E(K_x = \pm\pi/2 + \delta K_x, K_y = \pm\pi/2 + \delta K_y) \approx E(\pi/2, \pi/2) + C(|\delta K_x| + |\delta K_y|)$, along the direction $(0,0)$ to (π,π).

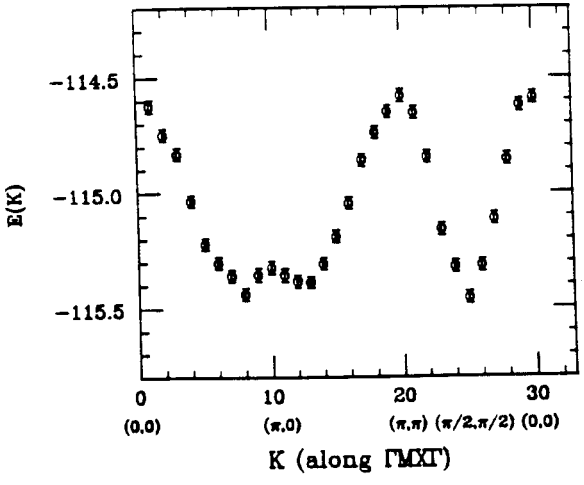

Fig.2. Dispersion curve, $E(\mathbf{K})$, plotted along the direction $\Gamma M X \Gamma$.

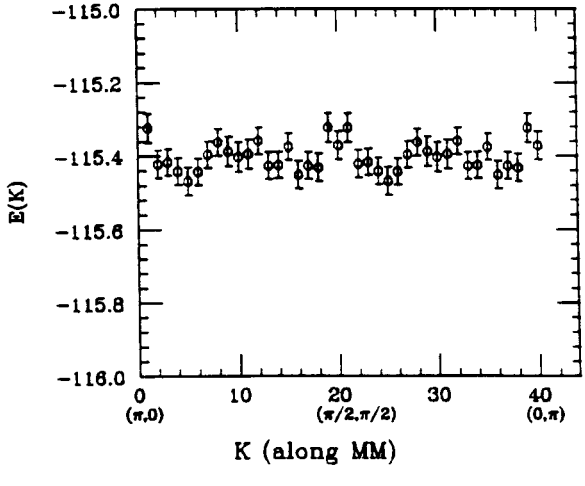

Fig.3. Dispersion curve, $E(\mathbf{K})$, plotted along the direction MM.

The bandwidth, obtained as the difference between $E(\pi/2, \pi/2)$ and $E(\pi, \pi)$, is plotted in Fig. 4; it decreases monotonically with J/t. On the ground of the

results obtained for the hole energy, we expect this picture to be correct when $J/t > 1$; large corrections are likely to arise for $J/t \leq 1$, due to effects arising from spin-hole-spin triplet correlations [15].

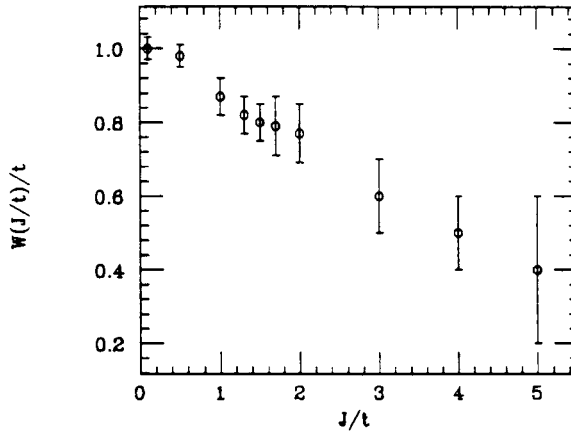

Fig.4. Bandwidth, W/t, plotted against J/t.

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6. References

1. P.W. Anderson, Science **235**,1196(1987).
2. F.C. Zhang and T.M. Rice, Phys. Rev. **37**,3759(1988).
3. E. Kaxiras and E. Manousakis, Phys. Rev. B **38**,866(1988).
4. E. Dagotto et. al., NSF-ITP-89-74, May 1989.
5. B. Shraiman and E. Siggia, Phys. Rev. Lett. **60**,740(1988).
6. B. Shraiman and E. Siggia, Phys. Rev. Lett. **61**,467(1988).
7. C. Kane, P. Lee and N. Read, Phys. Rev. B **39**,6880(1989); C. Gros and M. Johnson, preprint.
8. G.A. Thomas et. al., Phys. Rev. Lett. **61**,1313(1988).
9. R.P. Feynman and M. Cohen, Phys. Rev. **102**,1189(1956).
10. T. Matsubara and H. Matsuda, Prog. Theor. Phys., **16**,569(1956).
11. W. Marshall, Proc. Roy. Soc. London A **232**,48(1955).
12. D.A. Huse and V. Elser, Phys. Rev. Lett. **60**,2531(1988).
13. E. Manousakis, Phys. Rev. B **40**,4904(1989); Z. Liu and E. Manousakis, in press.
14. E. Manousakis and V.R. Pandharipande, Phys. Rev. B **33**,150(1986)
15. M. Boninsegni and E. Manousakis, to be published